

CLAIMS:

1. A three-dimensional quantitative structure-activity relationship method of extracting and visually
5 displaying characteristics of a compound based on the atomic coordinates of plural molecules superposed within a virtual space, comprising:

a process A of superposing plural molecules in a virtual space;

10 a process B of performing cluster analysis of the atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented points;

15 a process C of calculating interactions between the respective atoms of said plural molecules thus superposed and said represented points; and

a process D of statistically analyzing said interactions,

20 wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the respective atoms contained in said plural molecules thus superposed in said virtual space;

25 a second process B2 of calculating interatomic distances between each atom and other atoms and identifying

the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

5 a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined
10 threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

15 a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

2. A three-dimensional quantitative structure-
20 activity relationship method of extracting and visually displaying characteristics of a compound based on the atomic coordinates of plural molecules superposed within a virtual space, comprising:

a process A of superposing plural molecules in a
25 virtual space;

a process B of performing cluster analysis of the atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented points;

5 a process C of calculating interactions between the respective atoms of said plural molecules thus superposed and said represented points; and

a process D of statistically analyzing said interactions,

10 wherein said process B of cluster analysis further comprises:

a process B1 of, when said molecules thus superposed in said virtual space include a ring structure or functional group, generating an imaginary atom at a position representing said ring structure or functional group when needed;

a process B2 of calculating interatomic distances between each atom and other atoms as for all atoms in said virtual space including said imaginary atom and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two

atoms in the weighted average coordinates of said two atoms to delete, when thus calculated shortest interatomic distance is equal to or smaller than a predetermined threshold value;

5 a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

10 a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

3. The three-dimensional quantitative structure-activity relationship method of claim 1 or 2, wherein said
15 interactions calculated during said process C include at least one of steric interactions, electrostatic interactions and hydrophobic interactions.

4. A program for a three-dimensional quantitative
20 structure-activity relationship method of extracting and visually displaying characteristics of a compound based on the atomic coordinates of plural molecules superposed within a virtual space, said program making a computer execute:

25 a process A of superposing plural molecules in a

virtual space;

a process B of performing cluster analysis of the atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented
5 points;

a process C of calculating interactions between the respective atoms of said plural molecules thus superposed and the represented points; and

a process D of statistically analyzing said
10 interactions,

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the respective atoms contained in said plural molecules
15 thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the
20 shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said
25 two atoms to delete, when thus calculated shortest

interatomic distance is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said
5 second process B2 including said atoms formed during said third process B3; and

a fifth process B5 of terminating said process B when thus calculated shortest interatomic distance is exceeds said predetermined threshold.

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5. A program for a three-dimensional quantitative structure-activity relationship method of extracting and visually displaying characteristics of a compound based on the atomic coordinates of plural molecules superposed
15 within a virtual space, said program making a computer execute:

a process A of superposing plural molecules in a virtual space;

a process B of performing cluster analysis of the
20 atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions between the respective atoms of said plural molecules thus superposed
25 and the represented points; and

a process D of statistically analyzing said interactions,

wherein said process B of cluster analysis further comprises:

5 a first process B1 of, when said molecules thus superposed in said virtual space include a ring structure or functional group, generating an imaginary atom at a position which represents said ring structure or functional group when needed;

10 a second process B2 of, as for all atoms in said virtual space including said imaginary atom, calculating interatomic distances with other atoms and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the
15 shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said
20 two atoms to delete, when thus calculated shortest interatomic distance is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said
25 second process B2 including said atoms formed during said

third process B3; and

a fifth process B5 of terminating said process B when thus calculated shortest interatomic distance is exceeds said predetermined threshold.

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6. The program of claim 4 or 5, wherein said interactions calculated during said process C include at least one of steric interactions, electrostatic interactions and hydrophobic interactions.

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